

2,4,6-Tricyano-1,3,5-triazine
7615-57-8 | DTXSID00274764

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 123 °C

Global applicability domain: Outside

Local applicability domain index: 2.34e-01

Confidence level: 4.50e-01

Nearest Neighbors from the Training Set

Image not found

2,4,6-Tricyano-1,3,5-triazine

Measured: 119

Predicted: 123

Image not found

6-Cyanopurine

Measured: 188

Predicted: 164

Image not found

1,1'-Diazene-1,2-diyl
dicyclohexanecarbonitrile

Measured: 116

Predicted: 115

Image not found

2,2'-Azobis(2-methylbutanenitrile)

Measured: 50.0

Predicted: 61.7

Image not found

Azapropazone

Measured: 247

Predicted: 214